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SIMSEA data management and dissemination

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Adolf Stips

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SIMSEA's tools and results

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Acknowledgements

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Abstract

Over the course of its two years, the "Scenario simulations of the changing Black Sea ecosystem" H2020-MSCA-IF-2014 project No 660841 (SIMSEA) produce a number of scientific results of the Black Sea dynamics and ecosystem evaluation. The report addresses a key information for the data management as it is already planned in the SIMSEA's Data Management Plan (DMP). Evidence has been gathered on the dissemination of data produced by the SIMSEA project. The data management and dissemination follows the Horizon 2020 Work Program 2016 guidelines. The purpose of this deliverable is to support the data management life cycle for all data that is processed or generated by the project. It provides an outline of the data types the project have generated, whether and how data can be exploited or made accessible for verification and re-use, and how it will be curated and preserved.
Keywords: SIMSEA, data management, dissemination, data types, data access and sharing

1. Introduction

This report implements SIMSEAS Dissemination Work Plan and DMP by describing how the SIMSES research data is managing. More specifically, it describes what data is shared, any associated metadata, how the data is made available, and how it will be preserved.

The report follows thoroughly the SIMSEAS DMP and "Guidelines on Data Management in Horizon 2020" stating that scientific generated research data will be easily:

- Discoverable
- Accessible
- Assessable and intelligible
- Useable beyond the original purpose for which it was collected
- Interoperable to specific quality

The report is organised as follows. Section 2 contains a brief clarification of the scientific publications and project deliverables, as well as ease of access. In section 3 data management activities aiming at sharing the results of numerical simulations are presented. While in section 4, tools accompanying SIMSEAS results and their dissemination are discussed. Communication activities are listed in section 5.

2. Scientific publications

Three technical reports, namely Miladinova-Marinova et al. (2016a) and Miladinova et al. (2016 b and c), which cover the implementation of the SIMSEA project and its deliverables have been published. The SIMSEAS's hydrodynamic model has been validated against independent measured/calculated temperature and salinity fields in Miladinova-Marinova et al. (2016a). A new Black Sea Ecosystem Model (BSEM) is linked via the Framework for Aquatic Biogeochemical Models (FABM,) with the hydrodynamic model. The coupled SIMSEA physical-ecosystem modelling tool has been calibrated for the Black Sea runs. How the quality of forcing data affects the SIMSEA results and an analysis the effect of meteorological forcing is presented in Miladinova et al. (2016 b). The atmospheric forcing capable to assess the potential changes in the Black Sea ecosystem is identified. In Miladinova et al. (2016 c) long-term hindcast scenarios with and without river nutrient loads are compared and discussed.

Open access to scientific publications has been ensured in order to have free of charge online access for users. Technical reports presenting the project results are deposited into the JRC Publications Repository (http://publications.jrc.ec.europa.eu/repository/). The JRC Publications Repository is an online service giving access to data about research publications produced by the European Commission's Joint Research Centre. It provides access to a full-text publication. A keyword for easy discovery and identification includes the project acronym SIMSEA.

An article entitled "Black Sea thermohaline properties: Long-term trends and variations" by S. Miladinova, A. Stips, E. Garcia-Gorriz and D. Macias Moy is submitted for publication in open access journal.

3. Results of numerical simulations

All numerical data produced during implementation of SIMSEA project consists of output of 3D hydrodynamic model or output of a coupled hydrodynamic-biogeochemical model.

3.1 Data types

Table 1. SIMSEA output data types

Data source	Water column profiles	Spatial coverage/ resolution	Temporal coverage/ frequency	Units
Hydrodynamic output	Temperature	27.8°E - 42°E and 40.8°N – 47.2°N	1960 – 2015 Monthly mean	°C
	Salinity	27.8°E - 42°E and 40.8°N – 47.2°N	1960 – 2015 Monthly mean	‰
Biogeochemical output	Oxygen	27.8°E - 42°E and 40.8°N – 47.2°N	2000 – 2015 Monthly mean	mmol O_2 m^{-3}
	Chlorophyll a	27.8°E - 42°E and 40.8°N – 47.2°N	2000 – 2015 Monthly mean	mg Chla m^{-3}

In Table 1 are listed the variables (water column profiles) that are produced by the SIMSEA project and to which an open access is provided. An example for the temperature and salinity vertical profiles, which can be obtained from the hydrodynamic output, is given in Figure 1. While in Fig. 2 are given the corresponding oxygen (mmol O_2 m^{-3}) and chlorophyll a (mg Chla m^{-3}) profiles from the surface to 200 m depth in different basin locations. SIMSEA data possesses high horizontal resolution (2 min longitude x 2 min latitude) that comprises of 423x172 horizontal data points. Illustrations of the horizontal maps that are possible to be plotted by extracting SIMSEA data are shown in Figs. 3 and 4, where surface salinity and chlorophyll a fields are plotted in September 2002.

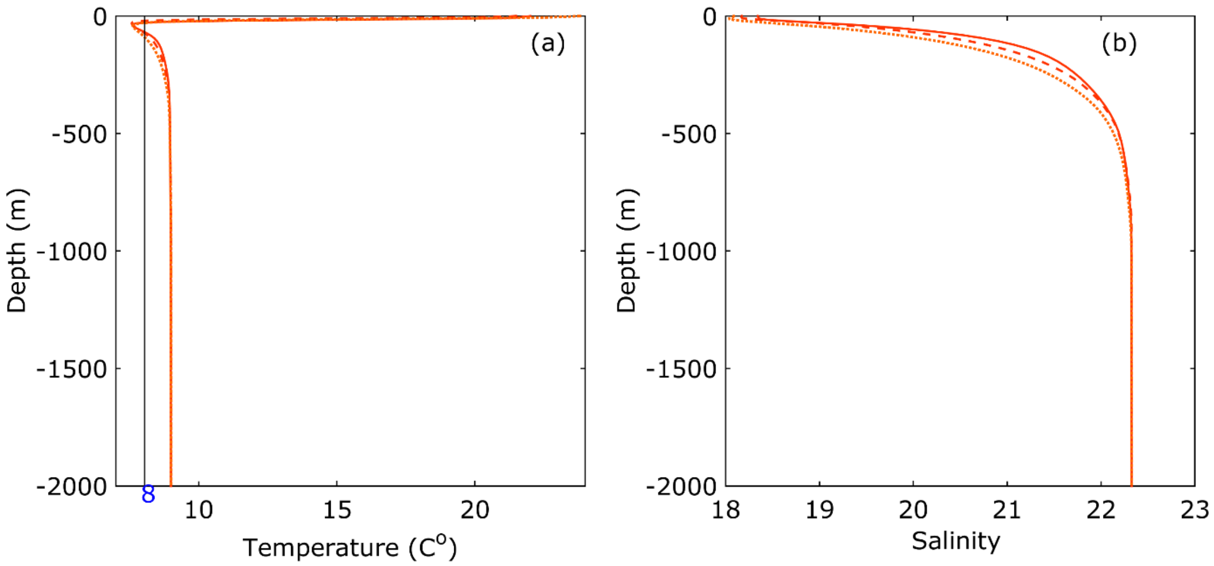

Figure. 1 Typical vertical (a) temperature and (b) salinity profiles in September from the Black Sea deep basin interior.

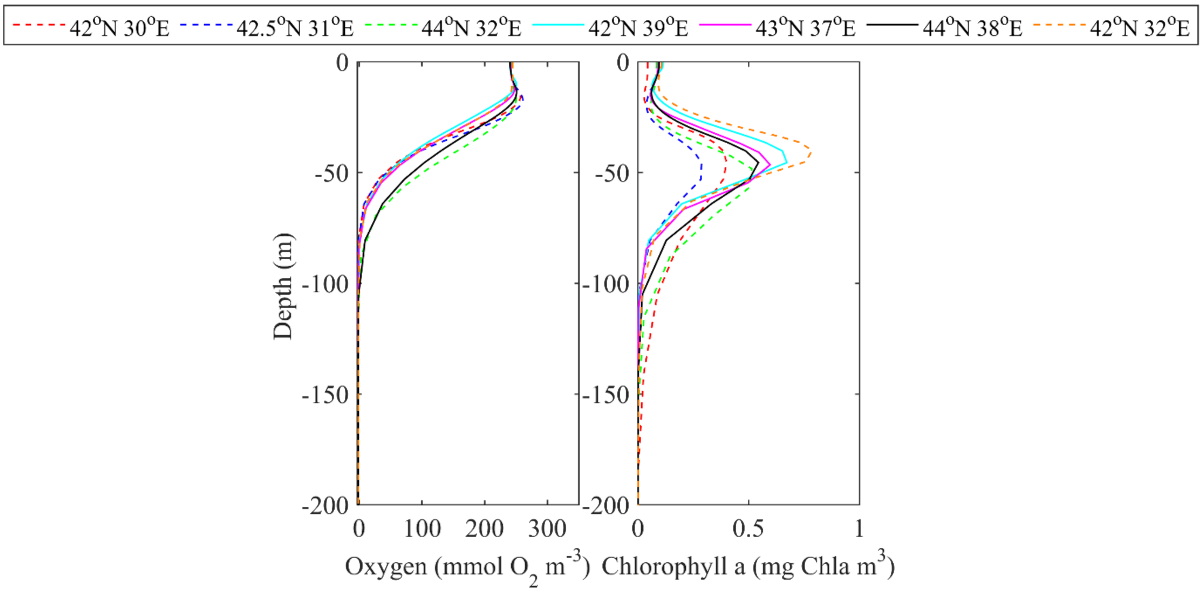

Figure. 2 Typical vertical oxygen (mmol O_2 m^{-3}) and chlorophyll a (mg Chla m^{-3}) profiles in September from the several Black Sea locations.

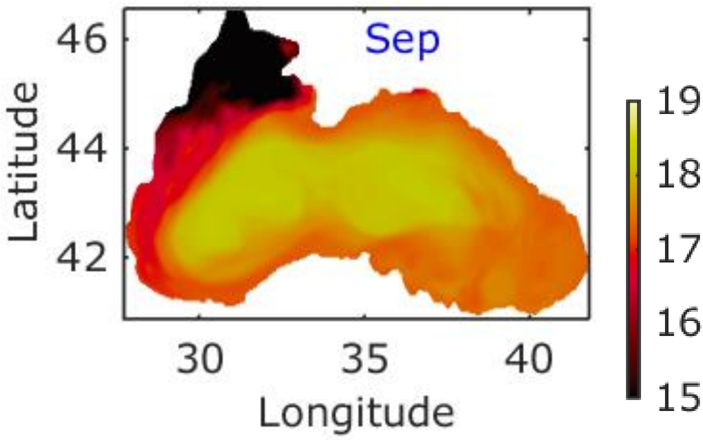

Figure 3. Surface salinity in September 2002.

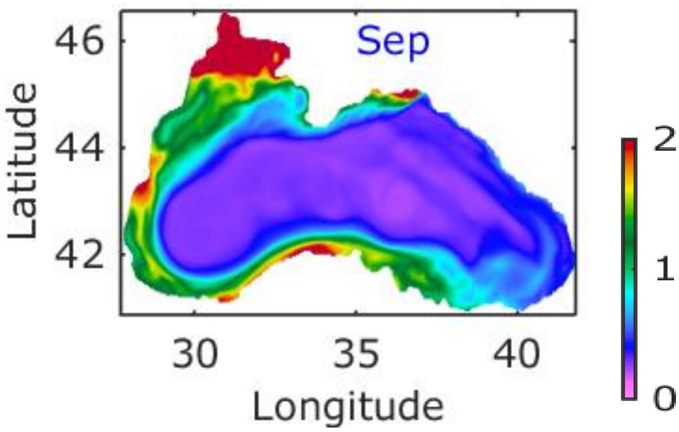

Figure 4. Surface chlorophyll (mg Chl m^{-3}) in September 2002.

3.2 Data storage and access

All numerical data produced will be uploaded on the Marine Geoportal that contains biological and physical variables generated from both hydrodynamic models and satellite remote sensing. Environmental Marine Information System (EMIS – European Seas) (http://mcc.jrc.ec.europa.eu/emis/) enable the user to conduct regional assessments. The EMIS marine geo-database is available for direct http download.

SIMSEA's results consist of individual downloadable NetCDF files covering the full Black Sea geographic extent (27.8°E - 42°E and 40.8°N – 47.2°N). The NetCDF file name structure and metadata file names are given in Table 2. All files can be downloaded from http://emis.jrc.ec.europa.eu/model/blacksea/. The NetCDF header includes information, in the form of a URL link, to where the metadata can be found.

Table 2. List of files stored in http://emis.jrc.ec.europa.eu/model/blacksea/

Data source	NetCDF file name	frequency	metadata
Temperature Salinity	EMIS_BLCK_TEMP_SALT_month_year.nc	month: from 01 to 12 year: from 1960 to 2015	EMIS_BLCK_MODEL_TEMP.xml EMIS_BLCK_MODEL_SALT.xml
Oxygen Chlorophyll a	EMIS_BLCK_TEMP_SALT_month_year.nc	month: from 01 to 12 year: from 2000 to 2015	EMIS_BLCK_MODEL_OXY.xml EMIS_BLCK_MODEL_CHL.xml

This data can be used by various groups like

- Researchers inside of academia

- Public bodies and agencies (e.g. the Commission on the Protection of the Black Sea Against Pollution (www.blacksea-commission.org), International Centre for Black Sea Study (www.icbss.org), Executive Environment Agency Bulgaria (eea.government.bg), etc.)

- Stakeholders/decision makers, mainly in support to the implementation of the Marine Strategy Framework Directive and the Strategy for the Danube Region.

4. Tools associated with SIMSEAS results

GETM, GOTM and FABM are the main tools used in SIMSEA simulations. They are written in Fortran and are provided as source codes (Table 3). To make the model useful the codes must be compiled to an executable program. The above codes are known to work on Linux/Unix, Mac and Windows computers provided a recent Fortran compiler. They have no external dependencies except for the NetCDF library.

Initialization files should include the following NetCDF files

- Black Sea's bathymetry
- Initial temperature and salinity fields

- River runoff, temperature, salinity and nutrient concentrations
- Meteorological forcing (air temperature, precipitation, wind, vapor pressure, and downward longwave and shortwave radiation)

The description of the initialization files and links are given in Table 4.

Table 3. SIMSEA model tools

Model	Tool	Metadata
3D Hydrodynamic	General Estuarine Ocean Model (GETM) General Ocean Turbulence Model (GOTM) Framework for Aquatic Biogeochemical Models (FABM)	Available via GPL2 Download from http://www.getm.eu/source-code/download/
3D Biogeochemical	Black Sea Specific Ecosystem Model (BSSM)	Available via GPL2 Download from https://github.com/fabm-model/code.git

Table 4. Input file description and access.

Input	File description	File Format	Primary data is available from
Initial data	Initial temperature and salinity fields Initial values of BSEM variables	NetCDF	http://www.ifremer.fr/medar http://sfp1.ims.metu.edu.tr/texts/database.htm
Topography	The Black Sea bathymetry	NetCDF	https://www.ngdc.noaa.gov/mgg/global/
River runoff	The Black Sea rivers flow rates Salinity and temperature of the rivers	NetCDF	http://www.daac.ornl.gov http://www.ifremer.fr/medar
Atmospheric data	Air temperature, precipitation, wind, vapour pressure, and downward longwave and shortwave radiation	NetCDF	http://www.esrl.noaa.gov
Water optical depth	The SeaWiFS ocean colour data	NetCDF	http://oceancolor.gsfc.nasa.gov/SeaWiFS
River load	Nutrient load from the rivers	NetCDF	http://www.ifremer.fr/medar

During the SIMSEA implementation period a new Black Sea bio-geochemical model (BSEM) has been in progress at the European Commission, DG Joint Research Centre, Directorate D – Sustainable Resources, Water and Marine Resources unit. The model has been developed using the Framework for Aquatic Biogeochemical Models (FABM – www.fabm.net). FABM was initiated during the Framework 7 project MEECE (http://www.meece.eu/) and has since then been maintained and further developed by Bolding & Bruggeman ApS (http://www.bolding-bruggeman.com). For a full description of FABM please visit the above given website or see in Bruggeman and Bolding (2014). FABM is open source and released under the GPL license. The goal is twofold: to bring the BSEM into the official, public FABM source code repository hosted at GitHub (http://www.github.com/fabm-model) and to assure the model quality both in terms of code quality and code performance. BSEM is available from the FABM code repository to the general public (see below the snapshot of the http://www.github.com/fabm-model webpage).

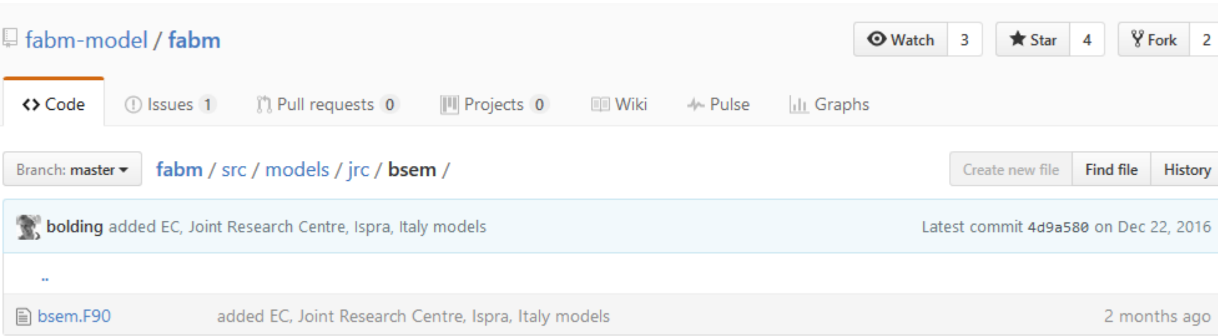

Figure 5. The snapshot of the http://www.github.com/fabm-model webpage.

The BSEM is a further development of a model developed by Oguz (Oguz et al., 2001) and is tailored specifically to include the processes important for the Black Sea pelagic ecosystem. The model includes 2 phytoplankton and 4 zooplankton types as well as PON, ammonium, nitrate, oxygen and hydrogen sulphate. The model consist of 468 code lines in a single Fortran source file – bsem.F90. The link to the source code in the repository is https://github.com/fabm-model/fabm/tree/master/src/models/jrc/bsem.

The model configuration including meta-data for all parameters is given in Figure 6. The file serves both as short documentation/description of the BSEM model but also as the actual configuration file used during a model simulation. The configuration file can always be kept up-to-date with the under-lying Fortran source code (the authoritative source for model definitions of variables, parameters and metadata) using the fabm_complete_yaml.py utility program available as part of FABM.

A setup example of the Black Sea modelling toolbox is stored in the JRC, namely, in the storage hpc-gw1.jrc.it/ACQUA/Black_Sea_GETM_BSEM_setup. The setup contains files used for the necessary technical installations, initial and boundary data. Several additional configuration files that are required for the model run are also provided (Garcia-Gorriz et al., 2016).

```
fabm-jrc-bsem.yaml (~/FABM/jrc/testcases) - VIM
require_initialization: true
instances:
  bsem:
    model: jrc/bsem
    check_conservation: true
    parameters:
      fluff: false             # include fluff layer (-), default = false
      sfl_ni: 0.0              # constant surface nitrate flux (mmol N/m2/d), default = 0.0
      sfl_am: 0.0              # mmolminimum phyto small concentration?? (mmol N/m3), default = 0.0
      pl0: 0.0225              # minimum phyto large concentration (mmol N/m3), default = 0.0225
      ps0: 0.0225              # minimum phyto small concentration (mmol N/m3), default = 0.0225
      alpha_l: 0.8             # initial slope of P-I curve for large phyto (-), default = 0.8
      alpha_s: 0.35            # initial slope of P-I curve for small phyto (-), default = 0.35
      sigma_l: 1.2             # maximum growth rate large phyto (1/d), default = 1.2
      sigma_s: 1.0             # maximum growth rate small phyto (1/d), default = 1.0
      beta_l: 0.0015           # initial slope of P-I curve for large phyto (-), default = 0.0015
      beta_s: 0.35             # initial slope of P-I curve for small phyto (-), default = 0.35
      kb: 0.01                 # shelf shading attenuation (-), default = 0.01
      ka_l: 0.3                # half-saturation for amm uptake large phyto (-), default = 0.3
      ka_s: 0.2                # half-saturation for amm uptake small phyto (-), default = 0.2
      kn_l: 0.5                # half-saturation for ni uptake large phyto (-), default = 0.5
      kn_s: 0.3                # half-saturation for ni uptake small phyto (-), default = 0.3
      mpl: 0.05                # mortality rate for large phyto (1/d), default = 0.005
      mps: 0.06                # mortality rate for small phyto (1/d), default = 0.006
      Q10: 2.0                 # temperature control of large phytoplankton growth (-), default = 2.0
      phyZ: 0.7                # Phytoplankton assimilation efficiency (-), default = 0.7
      g_zs: 0.8                # maximum grazing rate of zoo small (1/d), default = 0.8
      g_zl: 0.5                # maximum grazing rate of zoo large (1/d), default = 0.5
      g_zn: 0.5                # maximum grazing rate of noctiluca (1/d), default = 0.5
      g_zg: 0.15               # maximum grazing rate of gelatinous zoo (1/d), default = 0.15
      k_zs: 0.4                # half-sat cte for zoo small grazing (-), default = 0.4
      k_zl: 0.5                # half-sat cte for zoo large grazing (-), default = 0.5
      k_zn: 0.4                # half-sat cte for zoo noctiuca grazing (-), default = 0.4
      kn_zg: 0.25              # half-sat cte for zoo gelatinous grazing (-), default = 0.25
      mzs: 0.1                 # mortality rate of zoo small (1/d), default = 0.1
      mzl0: 0.25               # default mortality rate of zoo large (1/d), default = 0.25
      mzn: 0.15                # mortality rate of noctiluca (1/d), default = 0.15
      mnzg: 0.02               # mortality rate of gelatinous (1/d), default = 0.02
      mpzg0: 0.1               # default predation mortality rate of zoo gelatinous (1/d), default = 0.1
      mu_zs: 0.06              # excretion rate of zoo small (1/d), default = 0.06
      mu_zl: 0.05              # excretion rate of zoo large (1/d), default = 0.05
      mu_zn: 0.06              # excretion rate of zoo noctiluca (1/d), default = 0.06
      mu_zg: 0.08              # excretion rate of zoo gelatinous (1/d), default = 0.08
      epsilon_n0: 0.05         # default remineralisation rate of dn (1/d), default = 0.05
      R0: 150.0                # half-sat value for dn remineralisation (-), default = 150.0
      w_dn: 5.0                # Detritus sedimentation rate (m/d), default = 5.0
      r_n0: 0.1                # default nitrification rate (1/d), default = 0.1
      r_a0: 0.01               # Amm oxid rate by nit (1/d), default = 0.1
      r_s: 0.001               # HS oxid rate by nit (1/d), default = 0.1
      r_o: 0.1                 # HS oxid rate by oxyg (1/d), default = 0.1
      r_u: 0.0                 # HS oxid rate by other procc (1/d), default = 0.1
      s1: 5.3                  # reduced nitrate/oxidized detritus (-), default = 5.3
      s2: 6.625                # oxygen production/recycled nitrogen (-), default = 6.625
      s4: 2.0                  # nitrification (-), default = 6.625
      lds: 3.5                 # rate of detritus sinking into sediment (m/d), default = 3.5
      lsd: 25.0                # rate of sediment resuspension (1/d), default = 25.0
      tau_crit: 0.07           # critical bottom stress (N /m2), default = 0.07
      lsa: 0.001               # rate of sediment mineralisation (1/d), default = 0.001
      bsa: 0.15                # temperature control of sediment mineralisation (1/deg C), default = 0.15
      pvel_c: 4.5              # A constant for adjusting oxygen flux (-), default = 3.5
      temp_bio_high: 25.0      # Upper temperature control of biological reactions (deg C), default = 20.0
      temp_bio_low: 5.0        # Lower temperature control of biological reactions (deg C), default = 5.0
      par_lim: 75.0            # PAR limitation for photo inhibition (W/m**2), default = 75.0
      temp_zg_lim: 16.0        # Gelationous zooplankton critical temperature (deg C), default = 16.0
      ox_zoop_grazing: 200.0   # Oxygen control for zooplankton grazing (mmol O2/m3), default = 200.0
      ox_min: 0.05             # Oxygen minimum allowed value (mmol O2/m3), default = 0.05
      ox_lim_exc: 300.0        # Oxygen control for zooplankton excretion (mmol O2/m3), default = 300.0
      ox_suboxic: 10.0         # Oxygen control for suboxic conditions (mmol O2/m3), default = 10.0
      zl_pred_lost: 1.0        # Fraction of Zl lost by predation (-), default = 0.5
    initialization:
      pl: 0.0045               # PhytoLarge (mmol N/m**3)
      ps: 0.0045               # PhytoSmall (mmol N/m**3)
      zs: 0.0025               # MicroZoo (mmol N/m**3)
      zl: 0.0025               # MesoZoo (mmol N/m**3)
      zn: 0.0025               # Noctiluca (mmol N/m**3)
      zg: 0.0025               # Mnemiopsis (mmol N/m**3)
      dn: 0.07                 # detritus (mmol N/m**3)
      am: 0.07                 # ammonium (mmol N/m**3)
      ni: 4.5                  # nitrate (mmol N/m**3)
      o2: 350.0                # oxygen (mmol O2/m**3)
      hs: 4.5                  # hydrogen sulfide (mmol HS/m**3)
~
                                                              1,1           All
```


Figure 6. The Black Sea Ecosystem Model configuration file in YAML format.

5. Communications

Scientific results of the SIMSEA implementation have been communicated to a broad research community at the 4th International Conference on Oceanography & Marine Biology, July 18-19, 2016, Brisbane, Australia. The theme of the conference was "Discovering the Advances in Ocean Science and Marine Life". This event brought together an international mix of experts, researchers and decision makers both from academia and industry across the globe in the fields of Marine Sciences, Marine Biology, Marine Geology, Marine Oceanography, Marine ecology.

Communication with citizens about the Black Sea modelling tool and its benefits is planned for the second half of April 2017 when a public lecture will be given at the Institute of Mechanics, Bulgarian Academy of Science, Sofia. The research-based knowledge will be disseminated to a broad research community as well as to policy makers and public bodies and agencies outside of academia.

6. Conclusions

This report provides an overview of the data that SIMSEA project has been produced together with related data management and dissemination. The several different ways of data dissemination have been outlined. Actually they include free access publishing of SIMSEA deliverables, storage and free access to SIMSEA numerical data and tools, and communication with research community and citizens outside the academia. Software specifically developed within SIMSEA project has been released under the General Public License (GPL) to allow other research groups to reproduce the achieved results. The report includes information, in the form of a URL link, to where the data can be found and downloaded.

SIMSEA project does not consider personal data processing or other ethic issues.

The SIMSEA project puts a strong emphasis on the appropriate collection and publication of the data to be published, on metadata and storing all the information necessary for the optimal use and reuse of those datasets.

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List of abbreviations and definitions

BSEM: Black Sea Specific Ecosystem Model
Chla: Chlorophyll a
DMP: Data Management Plan
EMIS: Environmental Marine Information System
FABM: Framework for Aquatic Biogeochemical Models
GETM: General Estuarine Ocean Model
GPL: General Public License
GOTM: General Ocean Turbulent Model
JRC: Joint Research Centre
MC: Marie Curie
MSFD: Marine Strategy Framework Directive
NetCDF: Network Common Data Form
SIMSEA: Scenario simulations of the changing Black Sea ecosystem

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Figure. 2 Typical vertical oxygen (mmol O_2 m^{-3}) and chlorophyll a (mg Chla m^{-3}) profiles in September from the several Black Sea locations.

Figure 3. Surface salinity in September 2002.

Figure 4. Surface chlorophyll (mg Chl m^{-3}) in September 2002.

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